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Witzkeite: A new rare nitrate-sulphate mineral from a guano deposit at Punta de Lobos, Chile

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Abstract

Witzkeite, ideally $Na_4K_4Ca(NO_3)_2(SO_4)_4 \cdot 2H_2O$, is a new mineral found in the oxidation zone of the guano mining field at Punta de Lobos, Tarapacá region, Chile. It occurs as colorless, tabular crystals up to 140 μm in length, associated with dittmanite and nitratine. Witzkeite is colorless and transparent, with a white streak and a vitreous luster. It is brittle, with Mohs hardness 2 and distinct cleavage on {001}. Measured density is 2.40(2) g/cm^3, calculated density is 2.403 g/cm^3. Witzkeite is biaxial (–) with refractive indexes $\alpha = 1.470(5)$, $\beta = 1.495(5)$, $\gamma = 1.510(5)$, measured $2V = 50–70°$. The empirical composition is (electron microprobe, mean of five analyses, H_2O, CO_2, and N_2O_5 by gas chromatography; wt%): Na_2O 12.83, K_2O 22.64, CaO 7.57, FeO 0.44, SO_3 39.96, N_2O_5 12.7, H_2O 4.5, total 100.64; CO_2 was not detected. The chemical formula, calculated based on 24 O, is: $Na_{3.40}K_{3.95}Ca_{1.11}Fe_{0.05}(NO_3)_{1.93}(SO_4)_{4.10}(H_{4.10}O_{1.81})$. Witzkeite is monoclinic, space group $C2/c$, with unit-cell parameters: $a = 24.902(2)$, $b = 5.3323(4)$, $c = 17.246(1)$ Å, $\beta = 94.281(7)°$, $V = 2283.6(3)$ Å^3 ($Z = 4$). The crystal structure was solved using single-crystal X-ray diffraction data and refined to $R_1(F) = 0.043$. Witzkeite belongs to a new structure type and is noteworthy for the very rare simultaneous presence of sulfate and nitrate groups. The eight strongest X-ray powder-diffraction lines [d in Å (I in %) (h k l)] are: 12.38 (100) (2 0 0), 4.13 (19) (6 0 0), 3.10 (24) (8 0 0), 2.99 (7) ($\overline{8}$ 0 2), 2.85 (6) (8 0 2), 2.69 (9) ($\overline{7}$ 1 3), 2.48 (12) (10 0 0), and 2.07 (54) (12 0 0). The IR spectrum of witzkeite was collected in the range 390–4000 cm^{-1}. The spectrum shows the typical bands of SO_4^{2-} ions (1192, 1154, 1116, 1101, 1084, 993, 634, and 617 cm^{-1}) and of NO_3^- ions (1385, 1354, 830, 716, and 2775 cm^{-1}). Moreover, a complex pattern of bands related to H_2O is visible (bands at 3565, 3419, 3260, 2405, 2110, 1638, and 499 cm^{-1}). The IR spectrum is discussed in detail.

Keywords: Witzkeite, new mineral, guano, crystal structure, sulfate, nitrate, IR spectroscopy